

Anti-forcing numbers of perfect matchings of graphs

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Abstract

We define the anti-forcing number of a perfect matching M of a graph G as the minimal number of edges of G whose deletion results in a subgraph with a unique perfect matching M , denoted by $af(G, M)$. The anti-forcing number of a graph proposed by Vukičević and Trinajstić in Kekulé structures of molecular graphs is in fact the minimum anti-forcing number of perfect matchings. For plane bipartite graph G with a perfect matching M , we obtain a minimax result: $af(G, M)$ equals the maximal number of M -alternating cycles of G where any two either are disjoint or intersect only at edges in M . For a hexagonal system H , we show that the maximum anti-forcing number of H equals the Fries number of H . As a consequence, we have that the Fries number of H is between the Clar number of H and twice. Further, some extremal graphs are discussed.

Keywords: Graph; Hexagonal system; Perfect matching; Forcing number; Anti-forcing number; Fries number.

1 Introduction

We only consider finite and simple graphs. Let G be a graph with vertex set $V(G)$ and edge set $E(G)$. A perfect matching or 1-factor M of a graph G is a set of edges of G such that each vertex of G is incident with exactly one edge in M .

A Kekulé structure of some molecular graph (for example, benzenoid and fullerene) coincides with a perfect matching of a graph. Randić and Klein [14, 20] proposed the

innate degree of freedom of a Kekulé structure, i.e. the least number of double bonds can determine this entire Kekule structure, nowadays it is called the forcing number by Harary et al. [13].

A *forcing set* S of a perfect matching M of G is a subset of M such that S is contained in no other perfect matchings of G . The *forcing number* of M is the smallest cardinality over all forcing sets of M , denoted by $f(G, M)$. An edge of G is called a *forcing edge* if it is contained in exactly one perfect matching of G . The *minimum* (resp. *maximum*) *forcing number* of G is the minimum (resp. maximum) value of forcing numbers of all perfect matchings of G , denoted by $f(G)$ (resp. $F(G)$). In general to compute the minimum forcing number of a graph with the maximum degree 3 is an NP-complete problem [3].

Let M be a perfect matching of a graph G . A cycle C of G is called an *M -alternating cycle* if the edges of C appear alternately in M and $E(G) \setminus M$.

Lemma 1.1. [2, 22] *A subset $S \subseteq M$ is a forcing set of M if and only if each M -alternating cycle of G contains at least one edge of S .*

For planar bipartite graphs, Pachter and Kim obtained the following minimax theorem by using Lucchesi and Younger's result in digraphs [18].

Theorem 1.2. [19] *Let M be a perfect matching in a planar bipartite graph G . Then $f(G, M) = c(M)$, where $c(M)$ is the maximum number of disjoint M -alternating cycles of G .*

A hexagonal system (or benzenoid) is a 2-connected finite plane graph such that every interior face is a regular hexagon of side length one. It can also be formed by a cycle with its interior in the infinite hexagonal lattice on the plane (graphene). A hexagonal system with a perfect matching is viewed as the carbon-skeleton of a benzenoid hydrocarbon.

Let H be a hexagonal system with a perfect matching M . A set of *disjoint M -alternating hexagons* of H is called an *M -resonant set*. A set of M -alternating hexagons of H (the intersection is allowed) is called an *M -alternating set*. A maximum resonant set of H over all perfect matchings is a *Clar structure* or *Clar set*, and its size is the *Clar number* of H , denoted by $cl(H)$ (cf. [12]). A Fries set of H is a maximum alternating set of H over all perfect matchings and the Fries number of H , denoted by $Fries(H)$, is the size of a Fries set of H . Both Clar number and Fries number can measure the stability of polycyclic benzenoid hydrocarbons [1, 6].

Theorem 1.3. [28] *Let H be a hexagonal system. Then $F(H) = cl(H)$.*

In this paper we consider the anti-forcing number of a graph, which was previously defined by Vukićević and Trinajstić [26,27] as the smallest number of edges whose removal results in a subgraph with a single perfect matching (see refs [5, 8, 9, 15, 30] for some researches on this topic). By an analogous manner as the forcing number we define the anti-forcing number, denoted by $af(G, M)$, of a perfect matching M of a graph G as the minimal number of edges not in M whose removal to fix a single perfect matching M of G . We can see that the anti-forcing number of a graph G is the minimum anti-forcing number of all perfect matchings of G . We also show that the anti-forcing number has a close relation with forcing number: For any perfect matching M of G , $f(G, M) \leq af(G, M) \leq (\Delta - 1)f(G, M)$, where Δ denotes the maximum degree of G . For plane bipartite graph G , we obtain a minimax result: For any perfect matching M of G , the anti-forcing number of M equals the maximal number of M -alternating cycles of G any two members of which intersect only at edges in M . For a hexagonal system H , we show that the maximum anti-forcing number of H equals the Fries number of H . As a consequence, we have that the Fries number of H is between the Clar number of H and twice. Discussions for some extremal graphs about the anti-forcing numbers show the anti-forcing number of a graph G with the maximum degree three can achieve the minimum forcing number or twice.

2 Anti-forcing number of perfect matchings

An anti-forcing set S of a graph G is a set of edges of G such that $G - S$ has a unique perfect matching. The smallest cardinality of anti-forcing sets of G is called the *anti-forcing number* of G and denoted by $af(G)$.

Given a perfect matching M of a graph G . If C is an M -alternating cycle of G , then the symmetric difference $M \oplus C$ is another perfect matching of G . Here C may be viewed as its edge-set. A subset $S \subseteq E(G) \setminus M$ is called an anti-forcing set of M if $G - S$ has a unique perfect matching, that is, M .

Lemma 2.1. *A set S of edges of G not in M is an anti-forcing set of M if and only if S contains at least one edge of every M -alternating cycle of G .*

Proof. If S is an anti-forcing set of M , then $G - S$ has a unique perfect matching, i.e. M . So $G - S$ has no M -alternating cycles. Otherwise, if $G - S$ has an M -alternating cycle C , then the symmetric difference $M \oplus C$ is another perfect matching of $G - S$ different from

M , a contradiction. Hence each M -alternating cycle of G contains at least one edge of S . Conversely, suppose that S contains at least one edge of every M -alternating cycle of G . That is, $G - S$ has no M -alternating cycles, so $G - S$ has a unique perfect matching. \square

The smallest cardinality of anti-forcing sets of M is called the anti-forcing number of M and denoted by $af(G, M)$. So we have the following relations between the forcing number and anti-forcing number.

Theorem 2.2. *Let G be a graph with the maximum degree Δ . For any perfect matching M of G , we have*

$$f(G, M) \leq af(G, M) \leq (\Delta - 1)f(G, M).$$

Proof. Given any anti-forcing set S of M . For each edge e in S , let e_1 and e_2 be the edges in M adjacent to e . All such edges e in S are replaced with one of e_1 and e_2 to get another set S' of edges in M . It is obvious that $|S'| \leq |S|$. Further we claim that S' is a forcing set of M . For any M -alternating cycle C of G , by Lemma 2.1 C must contain an edge e in S . Then C must pass through both e_1 and e_2 . By the definition for S' , C contains at least one edge of S' . So Lemma 1.1 implies that S' is a forcing set of M . Hence the claim holds. So $f(G, M) \leq |S'| \leq |S|$, and the first inequality is proved.

Now we consider the second inequality. Let F be a minimum forcing set of M . Then $f(G, M) = |F|$. For each edge e in F , we choose all the edges not in M incident with one end of e . All such edges form a set F' of size no larger than $(\Delta - 1)|F|$, which is disjoint with M . We claim that F' is an anti-forcing set of M . Otherwise, Lemma 2.1 implies that $G - F'$ contains an M -alternating cycle C . Since each edge in F is a pendant edge of $G - F'$, C does not pass through an edge of F . This contradicts that F is a forcing set of M by Lemma 1.1. Hence $af(G, M) \leq |F'| \leq (\Delta - 1)|F|$. \square

Lemma 2.3. $af(G) = \min\{af(G, M) : M \text{ is a perfect matching of } G\}$.

By the definitions the above result is immediate. Hence we may say, $af(G)$ is the *minimum anti-forcing number* of G . Whereas,

$$Af(G) := \max\{af(G, M) : M \text{ is a perfect matching of } G\}$$

is the *maximum anti-forcing number* of G .

The following is an immediate consequence of Theorem 2.2.

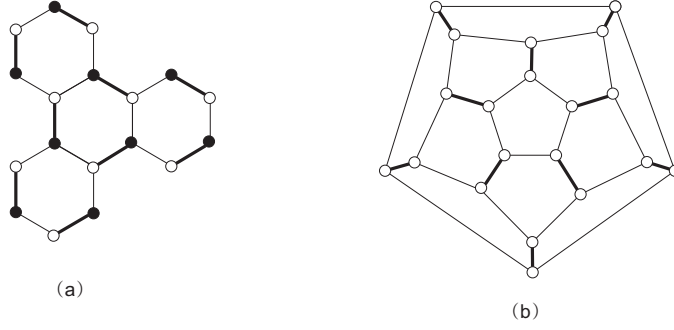


Figure 1: (a) Triphenylene, (b) Dodecahedron.

Corollary 2.4. *Let G be a graph with a perfect matching and the maximum degree Δ . Then*

$$f(G) \leq af(G) \leq (\Delta - 1)f(G), F(G) \leq Af(G) \leq (\Delta - 1)F(G).$$

Further, $\text{Spec}_f(G) := \{f(G, M) : M \text{ is a perfect matching of } G\}$ and $\text{Spec}_{af}(G) := \{af(G, M) : M \text{ is a perfect matching of } G\}$ are called the *forcing spectrum* [3] and the *anti-forcing spectrum* of G respectively. For example, $\text{Spec}_{af}(\text{Triphenylene}) = \{2, 3, 4\}$ and $\text{Spec}_f(\text{Triphenylene}) = \{1, 3\}$ (see Fig. 1(a)), $\text{Spec}_f(\text{Dodecahedron}) = \{3\}$ [31](see Fig. 1(b)). Randić and Vukićević [21, 25] computed the distributions of forcing numbers of Kekulé structures of C_{60} and C_{70} respectively.

For any given graph G with a perfect matching M , we now consider the anti-forcing number $af(G, M)$. If G has two M -alternating cycles that either are disjoint or intersect only at edges in M , then by Lemma 2.1 any anti-forcing set of M contains an edge of each one of such M -alternating cycles. Thus it naturally motivates us to propose a novel concept: a collection A of M -alternating cycles of G is called a *compatible M -alternating set* if any two members of A either are disjoint or intersect only at edges in M . Let $c'(M)$ denote the maximum cardinality of compatible M -alternating sets of G . By the above discussion we have the following immediate result.

Lemma 2.5. *For any perfect matching M of a graph G , we have $af(G, M) \geq c'(M)$.*

For plane bipartite graphs G we can show that the equality in the above lemma always holds. The vertices of G are colored with white and black such that any pair of adjacent vertices receive different colors. Such two color classes form a bipartition of G .

Theorem 2.6. *Let G be a planar bipartite graph with a perfect matching M . Then*

$$af(G, M) = c'(M).$$

To obtain such a minimax result we need a classical result of Lucchesi and Younger [18] about directed graphs; Its shorter proof was ever given by Lovász [16]. Let D be a finite directed graph. A *feedback set* of D is a set of arcs that contains at least one arc of each directed cycle of D .

Theorem 2.7 (Lucchesi and Younger). [18] *For a finite planar digraph, a minimum feedback set has cardinality equal to that of a maximum collection of arc-disjoint directed cycles.*

Proof of Theorem 2.6. First assign a specific orientation of G concerning M to obtain a digraph $\vec{G}(M)$: any edge in M is directed from white end to black end, and the edges not in M are directed from black ends to white ends. Obviously the M -alternating cycles of G corresponds naturally to directed cycles of its orientation. Then contract each edge of M in $\vec{G}(M)$ to a vertex (i.e. delete the edge and identify its ends) to get a new digraph, denoted by $\vec{G} \cdot M$. We can see that there is a one-to-one correspondence between the M -alternating cycles of G and directed cycles of $\vec{G} \cdot M$. That is, an M -alternating cycle of G becomes a directed cycle $\vec{G} \cdot M$, and a directed cycle of $\vec{G} \cdot M$ can produce an M -alternating cycle of G when each vertex is restored to an edge of M . So by Lemma 2.1 a subset $S \subseteq E(G) \setminus M$ is an anti-forcing set of M if and only if S is a feedback set of $\vec{G} \cdot M$. Hence $af(G, M)$ equals the smallest cardinality of feedback sets of $\vec{G} \cdot M$. On the other hand, a compatible M -alternating set of G corresponds to a set of arc-disjoint directed cycles of $\vec{G} \cdot M$. That implies that $c'(M)$ equals the maximum number of arc-disjoint directed cycles of $\vec{G} \cdot M$. Note that $\vec{G} \cdot M$ is a planar digraph. So Theorem 2.7 implies $af(G, M) = c'(M)$. \square

However, the equality in Lemma 2.5 does not necessarily hold in general. A counterexample is dodecahedron (see Fig. 1(b)); For this specific perfect matching marked by bold lines, it can be confirmed that there are at most three compatible alternating cycles, but its anti-forcing number is at least four.

3 Maximum anti-forcing number

In this section we restrict our consideration to a hexagonal system H with a perfect matching M . Without loss of generality, H is placed in the plane such that an edge-direction is vertical and the peaks (i.e. those vertices of H that just have two low neighbors, but no high neighbors) are black. An M -alternating cycle C of H is said to be *proper* (resp.

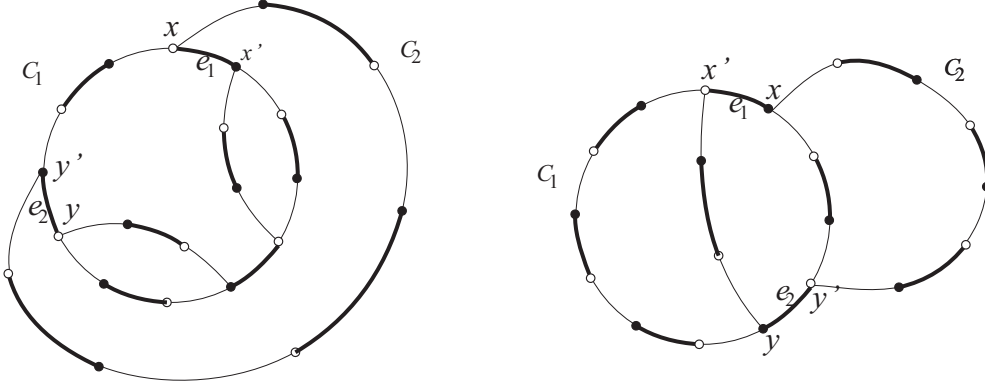


Figure 2: Two ways of crossing M -alternating cycles C_1 and C_2 (bold lines are edges in M).

improper) if each edge of C in M goes from white end to black end (resp. from black end to white end) along the clockwise direction of C . The boundary of H means the boundary of the outer face. An edge on the boundary is a boundary edge.

The following main result shows that the maximum anti-forcing number equals the Fries number in a hexagonal system.

Theorem 3.1. *Let H be a hexagonal system with a perfect matching. Then $Af(H) = Fries(H)$.*

Proof. Since any Fries set of H is a compatible M -alternating set A for some perfect matching M of H , we have that $Af(H) \geq Fries(H)$ from Theorem 2.6. So we now prove that $Af(H) \leq Fries(H)$. It suffices to prove that for a compatible alternating set A of H with $|A| = Af(H)$, we can find a Fries set F of H such that $|A| \leq |F|$.

Given any compatible M -alternating set A of H with a perfect matching M . Two cycles C_1 and C_2 in A are *crossing* if they share an edge e in M and the four edges adjacent to e alternate in C_1 and C_2 (i.e. C_1 enters into C_2 from one side and leaves from the other side via e). Such an edge e is said to be a crossing. For example, see Fig. 2. We say A is *non-crossing* if any two cycles in A are not crossing.

Claim 1. For any compatible M -alternating set A of H , we can find the corresponding non-crossing compatible M -alternating set A' of H such that $|A'| = |A|$.

Proof. Suppose A has a pair of crossing members C_1 and C_2 . In fact C_1 and C_2 have even number of crossings. Let e_1 and e_2 be two consecutive crossings, which are edges in M . So we may suppose along the counterclockwise direction C_2 from edge $e_1 = xx'$ enters into the interior of C_1 , then reaches the crossing $e_2 = yy'$. Note that x is the first vertex

of C_2 entering in C_1 and y' the first vertex of C_2 leaving from C_1 after x . For convenience, if a cycle C in H has two vertices s and t , we always denote by $C(s, t)$ the path from s to t along C clockwise. If C_1 is a proper M -alternating cycle and C_2 is an improper M -alternating cycle, let $C'_1 := C_1(y, x') + C_2(y, x')$ and $C'_2 := C_1(x', y) + C_2(x', y)$ (see Fig. 2(left)). If C_1 and C_2 both are proper (resp. improper) M -alternating cycles, let $C'_1 := C_1(y', x) + C_2(x, y')$ and $C'_2 := C_1(x, y') + C_2(y', x)$ (see Fig. 2(right)). In all such cases C_1 and C_2 in A can be replaced with C'_1 and C'_2 to get a new compatible M -alternating set of H and such a pair of crossings e_1 and e_2 disappeared. Since such a change cannot produce any new crossings, by repeating the above process we finally get a compatible M -alternating set A' of H that is non-crossing. It is obvious that $|A'| = |A|$. \square

For a cycle C of H , let $h(C)$ denote the number of hexagons in the interior of C . By Claim 1 we can choose a perfect matching M of H and a maximum compatible M -alternating set A satisfying that (i) $|A| = Af(H)$ and (ii) A is non-crossing, and $h(A) := \sum_{C \in A} h(C)$ is as minimal as possible subject to (i) and (ii). We call $h(A)$ the *h-index* of A .

By the above choice we know that for any two cycles in A their interiors either are disjoint or one contains the other one. Hence the cycles in A form a *poset* according to the containment relation of their interiors. Since each M -alternating cycle has an M -alternating hexagon in its interior (cf. [32]), we immediately obtain the following claim.

Claim 2. Every minimal member of A is a hexagon.

It suffices to prove that all members of A are hexagons. Suppose to the contrary that A has at least one non-hexagon member. Let C be a minimal non-hexagon member in A . Then C is an M -alternating cycle. We consider a new hexagonal system H' formed by C and its interior as a subgraph of H . Without loss of generality, suppose that C is a proper M -alternating cycle (otherwise, analogous arguments are implemented on right-top corner of H'). So we can find a substructure of H' in its left-top corner as follows.

We follow the notations of Zheng and Chen [33]. Let $S(i, j), 1 \leq i \leq m$ and $1 \leq j \leq n(i)$, be a series of hexagons on the boundary of H' as Fig. 3 that form a hexagonal chain and satisfy that neither B nor B' is contained in H' . We denote edges, if any, by $e(i, k), 1 \leq i \leq m$ and $1 \leq k \leq 2n(i)$, and by $f(i, j), 1 \leq i \leq m$ and $1 \leq j \leq n(i)$; and denote the hexagons (not necessarily contained in H') with both edges $f(i, j)$ and $e(i, 2j - 1)$, by $T(i, j), 1 \leq i \leq m$ and $1 \leq j \leq n(i)$ (see Fig. 3).

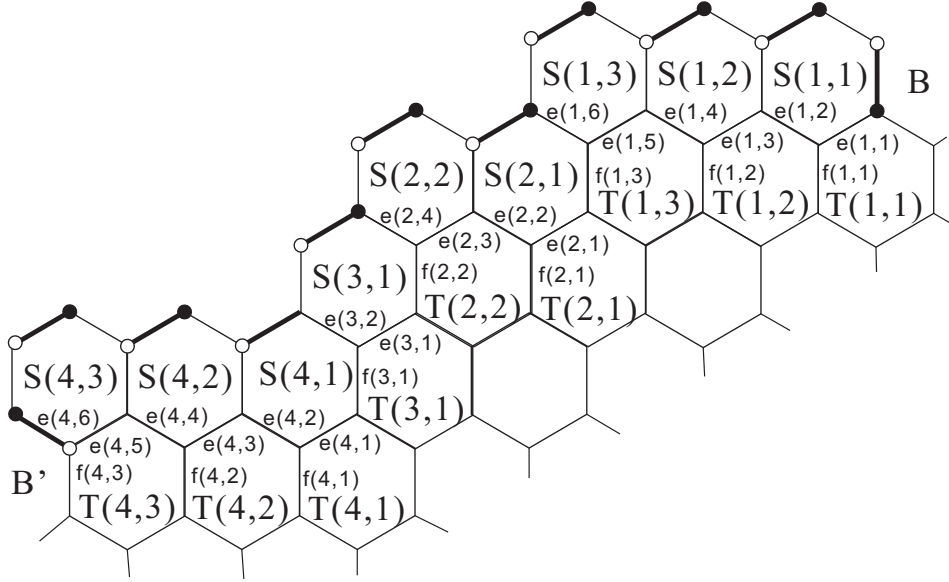


Figure 3: Illustration for the proof of Claim 3 (bold lines are edges in M , $m = 4, n(1) = 3, (n(2) = 2, n(3) = 1, n(4) = 3)$).

- Claim 3.** (a) $n(1) = 1$, and $m \geq 2$,
(b) $n(i) = 1$ or 2 for all $1 \leq i \leq m$,
(c) for all $1 \leq i \leq m$, $f(i, n(i)) \in M$, and
(d) if $n(i) = 2$, $2 \leq i \leq m$, then $S(i, 1) \in A$.

Proof. We now prove the claim by induction on i . We first consider $i = 1$. If $e(1, 2) \in M$, then $S(1, 1)$ is a proper M -alternating hexagon. So C in A can be replaced with $S(1, 1)$ to produce a new compatible M -alternating set A' . That is, $A' := (A \cup S(1, 1)) - \{C\}$, but $|h(A')| < |h(A)|$, a contradiction. So $e(1, 2) \notin M$, which implies that $f(1, 1) \in M$ and all edges $e(1, 3), e(1, 5), \dots, e(1, 2n(1) - 1)$ belong to M . Hence $S(2, 1)$ is a hexagon of H' and $m \geq 2$. If $n(1) \geq 2$, since the boundary C of H' is a proper M -alternating cycle, none of the edges $e(1, 2), e(1, 3), \dots, e(1, 2n(1))$ is a boundary edge of H' . In this case the cycle C can be replaced with $C \oplus S(1, n(1))$ to get another compatible M -alternating set with less index h -index than A , also a contradiction. Hence $n(1) = 1$. So the claim holds for $i = 1$.

Suppose $1 \leq i < m$ and Claim 3 holds for any integer $1 \leq i' \leq i$. We want to show that it holds for $i + 1$. There are two cases to be considered.

Case 1. $n(i) = 1$. Suppose that $n(i + 1) \geq 3$. If $e(i + 1, 2) \notin M$, then $e(i + 1, 3), e(i + 1, 5), \dots, e(i + 1, 2n(i) - 1)$ all belong to M . By an analogous argument as above, we have that $T(i + 1, 2), \dots, T(i + 1, n(i + 1)), S(i + 2, 1)$ are hexagons of H' , and C can be replaced

with $C \oplus S(i+1, n(i+1))$ to get another M -compatible alternating set with less h -index than h , also a contradiction. Hence $e(i+1, 2) \in M$. By the induction hypothesis we have $f(i, 1) \in M$, and $S(i+1, 1)$ is an M -alternating hexagon. If $e(i+1, 4) \notin M$, the similar contradiction occurs. So $e(i+1, 4) \in M$. We can see that none of members of A but C intersect $S(i+1, 1)$. Then $(A \cup \{S(i, 1), S(i+1, 1), S(i+2, 2)\}) - \{C\}$ is a compatible $M \oplus S(i+1, 1)$ -alternating set, which is larger than A , contradicting the choice of A . Hence $n(i+1) \leq 2$. If $n(i+1) = 1$, then $f(i+1, 1) \in M$. Otherwise, C in A would be replaced with $S(i+1, 1)$ to obtain a similar contradiction. If $n(i+1) = 2$, by the similar arguments we have that $e(i+1, 2) \in M$ and $f(i+1, 2) \in M$. So $S(i+1, 1) \in A$.

Case 2. $n(i) = 2$. Choose an integer i_0 with $1 \leq i_0 < i$ such that $n(i_0) = 1$, and $n(i_0 + 1) = n(i_0 + 2) = \dots = n(i) = 2$. By the induction hypothesis, we have that the right vertical edge of hexagon $S(i_0, 1)$ belongs to M , the hexagons $S(i_0 + 1, 1), S(i_0 + 2, 1), \dots, S(i, 1)$ are all proper M -alternating hexagons, which all belong to A , and $f(i, 2) \in M$. If $e(i+1, 2) \notin M$, then $f(i+1, 1) \in M$. We have that $n(i+1) = 1$; otherwise, $n(i+1) \geq 2$ and C would be replaced with $C \oplus S(i+1, n(i+1))$ to get another M -compatible alternating set with less h -index than A , also a contradiction. So suppose that $e(i+1, 2) \in M$. Then $S(i+1, 1)$ is a proper M -alternating hexagon. We claim that $n(i+1) = 2$ and $f(i+1, n(i+1)) \in M$. If $n(i+1) = 1$, then $e(i+1, 2)$ belongs to C . So C can be replaced with $S(i+1, 1)$ also to get a contradiction. Hence $n(i+1) \geq 2$. Suppose $e(i+1, 4) \in M$. Let $M' = M \oplus S(i+1, 1) \oplus S(i, 1) \oplus \dots \oplus S(i_0 + 1, 1)$. Then M' is a perfect matching of H so that $S(i+1, 2), S(i+1, 1), S(i, 2), S(i, 1), \dots, S(i_0 + 1, 2), S(i_0 + 1, 1), S(i_0, 1)$ are M' -alternating hexagons. Let $A' := (A \cup \{S(i+1, 2), S(i, 2), \dots, S(i_0 + 1, 2), S(i_0, 1)\}) - \{C, T(i, 2), \dots, T(i_0 + 1, 2)\}$. Then A' is a compatible M' -alternating set of H with $|A| < |A'|$, contradicting the choice for A . Hence $e(i+1, 4) \notin M$ and $f(i+1, 2) \in M$. If $n(i+1) \geq 3$, then $e(i+1, 5), e(i+1, 7), \dots, e(i+1, 2n(i+1) - 1)$ all belong to M , so C can be replaced with $C \oplus S(i+1, n(i+1))$ to get a similar contradiction. Hence $n(i+1) = 2$ and the claim holds. Further we have that $S(i+1, 1) \in A$.

Now we have completed the proof of Claim 3. \square

By Claim 3 we have that $f(m, n(m)) \in M$. That implies that $e(m, 2n(m)) \notin M$. So $S(m+1, 1)$ exists in H' , a contradiction. Hence each member of A is a hexagon. \square

Combining Theorems 1.3 and 3.1 with Corollary 2.4, we immediately obtain the following relations between the Clar number and Fries number.

Corollary 3.2. *Let H be a hexagonal system. Then $cl(H) \leq \text{Fries}(H) \leq 2cl(H)$.*

4 Some extremal classes

4.1 All-kink catahexes

Let H be a hexagonal system. The inner dual H^* of H is a plane graph: the center of each hexagon h of H is placed a vertex h^* of H^* , and if two hexagons of H share an edge, then the corresponding vertices are joined by an edge. H is called catacondensed if its inner dual is a tree. Further H is called *all-kink catahex* [13] if it is catacondensed and no two hexagons share a pair of parallel edges of a hexagons. The following result due to Harary et al. gives a characterization for a hexagonal system to have the Fries number (or the maximum anti-forcing number) achieving the number of hexagons.

Theorem 4.1. [13] *For a hexagonal system H with n hexagons, $Fries(H) \leq n$, and equality holds if and only if H is an all-kink catahex.*

An independent (or stable) set of a graph G is a set of vertices no two of which are adjacent. The independence number of G , denoted by $\alpha(G)$, is the largest cardinality of independent sets of G .

Theorem 4.2. *For an all-kink catahex H , $Af(H) = 2F(H)$ if and only if the inner dual H^* has a perfect matching.*

Proof. By Theorem 4.1, $Af(H)$ equals the number n of vertices of H^* . Note that any set of disjoint hexagons of H is a resonant set. By Theorem 1.3, $F(H) = cl(H) = \alpha(H^*)$. Since H^* is a bipartite graph, $\nu(H^*) + \alpha(H^*) = n$, where $\nu(H^*)$ denotes the matching number of H^* , the size of a maximum matching of H^* . So this equality implies the result. \square

For a hexagonal system H with a perfect matching M , let $fries(M)$ be the number of M -alternating hexagons of H . Then $Fries(H)$ is the maximal value of $fries(M)$ over all perfect matchings. The minimal value of $fries(M)$ over all perfect matchings M is called the *minimum fries number*, denoted by $fries(H)$. For an all-kink catahex, each hexagon has two choices for three disjoint edges, and just one's edges can be glued with other hexagons, so these three edges are called *fusing edges*. If a fusing edge is on the boundary, then an additive hexagon is glued along it to get a larger all-kink catahex.

A *dominating set* of a graph G is a set S of vertices of G such that every vertex not in S has a neighbor in S . An independent dominating set of G is a set of vertices of G

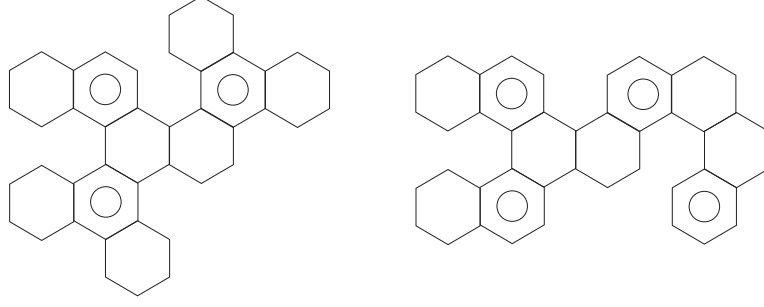


Figure 4: All-kink catahexes with the minimum forcing numbers 3 and 4

that is both dominating and independent in G [10]. The independent domination number of G , denoted by $i(G)$, is the minimum size of independent dominating sets of G . (For a survey on independent domination, see [10])

Theorem 4.3. *For an all-kink catahex H , $f(H) = i(H^*) = \text{fries}(H)$.*

Proof. For any perfect matching M of H , by Theorem 1.2 we have that $f(H, M) = c(M)$. Note that H has no interior vertices. Since each M -alternating cycle of H contains an M -alternating hexagon in its interior, $c(M)$ equals the maximum number of disjoint M -alternating hexagons of H . It is obvious that for a hexagon of H a non-fusing edge belongs to M if and only if the three non-fusing edges belong to M .

Choose a perfect matching M of H such that $f(H) = f(H, M)$. Let S be a maximum set of disjoint M -alternating hexagons of H and $S^* := \{h^* : h \in S\}$. Then $f(H) = |S^*|$. We claim that S^* is an independent dominating set of H^* . Let h be any hexagon of H not in S . If some hexagon h' of H adjacent to h has the three non-fusing edges in M , then $h' \in S$. Otherwise, h is an M -alternating hexagon. Since $h \notin S$ and S is maximum, some hexagon of H adjacent to h must belong to S . So the claim holds, and $f(H) \geq i(H^*)$. Conversely, given a minimum independent dominating set S^* of H^* . Construct a perfect matching M_0 of H as follows. The three non-fusing edges of each hexagon in S are chosen as edges of M_0 . For any hexagon of H not in S , a fusing edge that is a boundary edge or shared by the other hexagon not in S is also an edge of M_0 . So we can see that M_0 is a perfect matching of H and any hexagon of H not in S is not M_0 -alternating. Hence S is the maximum set of M_0 -alternating hexagons of H . So $i(H^*) = f(H, M_0) \geq f(H)$. Hence $i(H^*) = f(H)$.

According to the above construction, S is the set of all M_0 -alternating hexagons of H . Hence $f(H) = h(M_0) \geq \text{fries}(H)$. On the other hand, for any perfect matching M of H , $c(M) \leq \text{fries}(M)$, and thus $f(H) \leq \text{fries}(H)$. Both inequalities imply the second

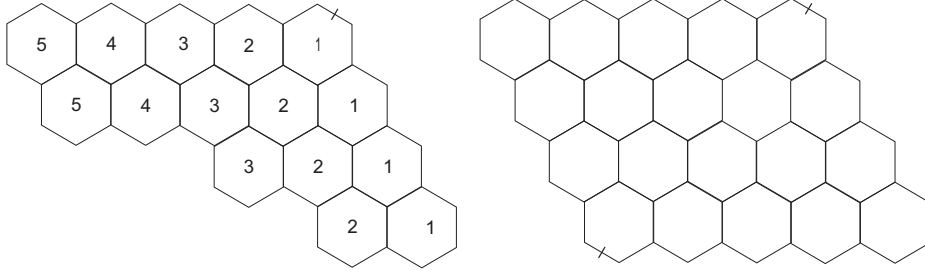


Figure 5: Truncated parallelograms $H(5, 5, 3, 2)$ and $H(5, 5, 5, 5)$ with anti-forcing edges marked by short lines.

equality. □

Beyer et al. [4] observed an algorithm of linear time to compute the independent domination number of a tree. So the minimum forcing number of all-kink catahexes can be computed in linear time. For example, Fig. 4 gives the minimum forcing numbers of two all-kink catahexes. But the anti-forcing number of an all-kink catahex may be larger than its minimum forcing number; for example, the triphenylene has the minimum forcing number 1 and the anti-forcing number 2 (see Fig. 1(a)).

4.2 $af(H) = 1, 2$

Li [15] gave the structure of hexagonal systems with an anti-forcing edge (i.e. an edge that itself forms an anti-forcing set). For integers $n_1 \geq n_2 \geq \dots \geq n_k$, let $H(n_1, n_2, \dots, n_k)$ be a hexagonal system with k horizontal rows of $n_1 \geq n_2 \geq \dots \geq n_k$ hexagons and last hexagon of each row being immediately below and to the right of the last one in the previous row, and we call it *truncated parallelogram* [7]; For example, See Fig. 5. In particular, $H(r, r, \dots, r)$ with $k \geq 2$ and $r \geq 2$ and $H(r)$ with $r \geq 2$ are parallelogram and linear chain respectively. Note that a truncated parallelogram can be placed and represented in other ways.

Theorem 4.4. [15] *Let H be a hexagonal system. Then $af(H) = 1$ if and only if H is a truncated parallelogram.*

Precisely, a single hexagon has six anti-forcing edges, a linear chain has four anti-forcing edges, and a parallelogram has two anti-forcing edges. A true truncated parallelogram has just one anti-forcing edge (see Fig. 5). In the following we will give a construction for hexagonal systems with the anti-forcing number 2.

Some necessary preliminary is needed. Let G be a connected plane bipartite graph. An edge of G is said to be *fixed single* (resp. *double*) if it belongs to no (resp. all) perfect matchings of G . G is *normal* or *elementary* if G has no fixed single edges. The non-fixed edges of G form a subgraph whose components are normal and thus 2-connected graphs, which are called *normal components* of G . Further, a normal component of G is called a *normal block* if it is formed by a cycle of G with its interior. A pendant vertex of a graph is a vertex of degree one, and its incident edge is a pendant edge.

Lemma 4.5. [17] *If a bipartite graph has a unique perfect matching, then it has a pair of pendant vertices with different colors.*

Lemma 4.6. [24] *Let H be a connected plane bipartite graph with a perfect matching. If all pendant vertices of G are of the same color and lie on the boundary, then G has at least one normal block. If G has a fixed single edge and $\delta(G) \geq 2$, then G has at least two normal blocks.*

The following result was first pointed out by Sachs and can be extended to bipartite graphs.

Lemma 4.7. [23] *Let H be a hexagonal system with a perfect matching. Let $E = \{e_1, e_2, \dots, e_r\}$ be a set of parallel edges of H such that e_i and e_{i+1} belong to the same hexagon and the e_1 and e_r are boundary edges. Then E is an edge-cut of H and $|E \cap M|$ is invariant for all perfect matchings M of H .*

Theorem 4.8. *Let H be a hexagonal system with a fixed single edge. Then $af(H) = 2$ if and only if H has exactly two normal components, which are both truncated parallelograms.*

Proof. By Lemma 4.6 H has at least two normal components. Such normal component is a hexagonal system with the anti-forcing number at least one. Note that the anti-forcing number of H equals the sum of the anti-forcing numbers of such normal components. Hence $af(H) = 2$ if and only if H has exactly two normal components, which are truncated parallelograms by Theorem 4.4. \square

Theorem 4.9. *Let H be a normal hexagonal system. Then $af(H) = 2$ if and only if H is not truncated parallelogram and H can be obtained by gluing two truncated parallelograms T_1 and T_2 along their boundary parts as a fused path P of odd length such that*

- (i) *an anti-forcing edge of T_1 remains on the boundary,*
- (ii) *the hexagons of each T_i with an edge of P form a linear chain or a chain with one*

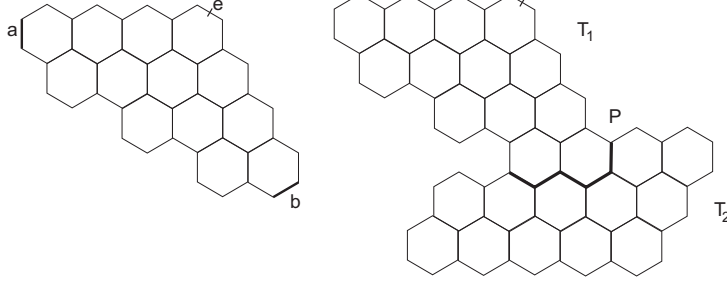


Figure 6: (a) A truncated parallelogram with specific edges a and b , (b) Gluing two truncated parallelograms.

kink (i.e. the inner dual is a path with exactly one turning vertex), and
(iii) *when the fused path P passes through edge b (or a) of T_1 , the hexagons of T_1 (resp. T_2) with an edge of P form a linear chain that is the last (or first) row of T_1 (resp. a chain with one kink). (see Fig. 6)*

Proof. Suppose that $af(H) = 2$. Then H has distinct edges e and e' such that $H' := H - e - e'$ has a unique perfect matching M . So by Lemma 4.5 H' has two pendant vertices with different colors. Then one of e and e' , say e , must be a boundary edge of H ; otherwise H' has at most one pendant vertex, a contradiction.

Claim 1. e has at least one end with degree two in H .

Otherwise, suppose that e has both ends with degree three. Then $H - e$ has the minimum degree two. If $H - e$ is 2-connected, it must be a hexagonal system other than truncated parallelogram, contradicting that $H - e$ has an anti-forcing edge e' . If $H - e$ has a cut edge, by Lemma 4.6 $H - e$ has at least two normal components. So $af(H - e) \geq 2$, also a contradiction, and Claim 1 holds.

So $H - e$ has a pendant vertex x . The edge e_0 between x and its neighbor belongs to all perfect matchings of $H - e$, and is thus anti-forced by e . Deleting the ends of this edge and incident edges, any pendant edges of the resulting graph also belong to all perfect matchings of $H - e$, such pendant edges are anti-forced by e . Repeating the above process, until to get a graph without pendant vertices, denoted by $H \ominus e$.

Claim 2. $H \ominus e$ is a truncated parallelogram with an anti-forcing edge e' .

If $H \ominus e$ is empty, then e is an anti-forcing edge of H , a contradiction. Otherwise, $H \ominus e$ has a perfect matching and the minimum degree two. Note that the interior faces of $H \ominus e$ are hexagons. By the similar arguments as the proof of Claim 1, we have that $H \ominus e$ is a hexagonal system with an anti-forcing edge e' . Hence Claim 2 holds.

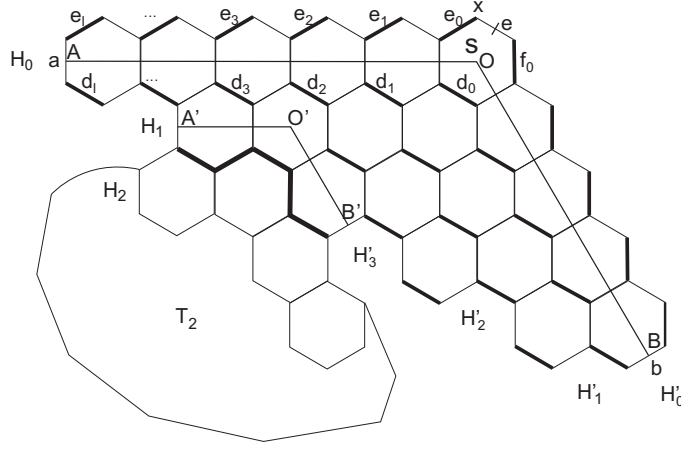


Figure 7: Illustration for the proof of Theorem 4.9 ($m = 1, m' = 3$)

Without loss of generality, suppose that edge e is from the left-up end x to the right-low end. Then e_0 is a slant edge. Let s be the hexagon with edge e , f_0 the vertical edge of s adjacent to e , d_0 the other edge of s parallel to e . From the center O of s draw a ray perpendicular to and away from f_0 (resp. e_0) intersecting a boundary edge a at A (resp. edge b at B) such that OA (resp. OB) only passes through hexagons of H . Let H_0 and H'_0 be the linear chains of H consisting of hexagons intersecting OA and OB ; See Fig. 7. By the similar reasons as Claim 1, we have the following claim.

Claim 3. It is impossible that H has not only hexagons adjacent above to H_0 but also hexagons adjacent right to H'_0 .

By Claim 3 we may suppose that H has no hexagons adjacent above to H_0 . Let e_1, e_2, \dots, e_l denote a series of edges in H_0 parallel to e_0 and above OA , d_1, d_2, \dots, d_l denote a series of edges in H_0 parallel to d_0 and below OA (see Fig. 7). Hence e_1, e_2, \dots, e_l are anti-forced by e in turn and thus belong to M .

Let H_1 be the graph consisting of the hexagons adjacent to H_0 and below it. If d_l is a boundary edge of H , then d_l, \dots, d_1, d_0 are further anti-forced by e and thus belong to M . So H_1 is a linear chain with an end hexagon in H'_0 , and thus H_1 has at most many hexagons as H_0 . Otherwise, by Lemma 4.7 we have that some vertical edges in H_1 are fixed single edges, contradicting that H is normal. In general, for $m \geq 0$ let H_{m+1} be the graph consisting of the hexagons adjacent to H_m and below it. If H_{m+1} has no hexagon adjacent left to the left end hexagon of H_m , by the same reasons as above we have that H_{m+1} is a linear chain with an end hexagon in H'_0 and the edges in H_{m+1} parallel to d_0 are anti-forced by e and thus belong to M . There are two cases to be considered.

Case 1. H has no hexagons adjacent right to H'_0 .

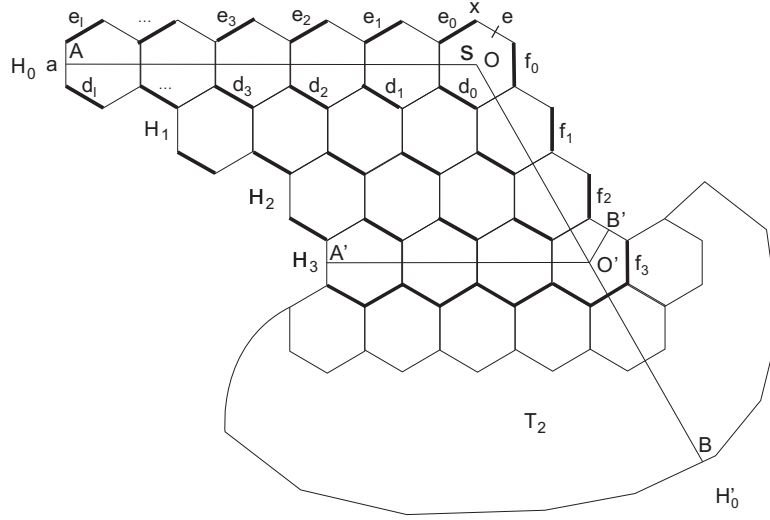


Figure 8: Illustration for the proof of Theorem 4.9 ($m = 3$)

In this case there must be an integer m such that for each $1 \leq i \leq m$, H_i is a linear chain with an end hexagon in H'_0 and H_i has at most many hexagons as H_{i-1} , but H_{m+1} has a hexagon adjacent left to the left end hexagon of H_m . Otherwise H is a truncated parallelogram, a contradiction. Along chain H'_0 , similarly as rows H_i we can define H'_j in turn and have the similar fact: there must be an integer m' such that for each $1 \leq j \leq m'$, H'_j is a linear chain with an end hexagon in H_0 and H'_j has at most many hexagons as H'_{j-1} , but $H'_{m'+1}$ has a hexagon adjacent below to the lowest hexagon of $H'_{m'}$ (see Fig. 7). Then H_m and $H'_{m'}$ have exactly one hexagon s' in common. Let O' be the center of s' , A' the center of the most-left vertical edge of H_m and B' the center of the lowest right edge of $H'_{m'}$. Hence $T_2 := H \ominus e$ is just a subhexagonal system lying in left-low side of the line $A'O'B'$. Let T_1 be the graph consisting of H_0, \dots, H_m and $H'_0, \dots, H'_{m'}$. It is obvious that T_1 is a truncated parallelogram, T_1 and T_2 intersect at a path of odd length, and statements (i) and (ii) holds.

Case 2. H has hexagons adjacent right to H'_0 . Let H''_0 be the graph consisting of hexagons of H adjacent right to H'_0 . Let m be the least integer such that H_m has the right end hexagon adjacent to a hexagon of H''_0 . Note that m may be zero. Let f_0, f_1, \dots, f_m be a series of vertical edges of H'_0 on its right side (see Fig. 8). Then the edges f_0, f_1, \dots, f_{m-1} are anti-forced by e and thus belong to M . If every H_i is a linear chain and H_i has no hexagons adjacent left to the left-end hexagon of H_{i-1} , then H''_0 is a linear chain that intersect H'_0 at a path of odd length, so $T_2 = H \ominus e$ must be a truncated parallelogram consisting of H''_0 and its right side. Otherwise, by analogous arguments we have that for

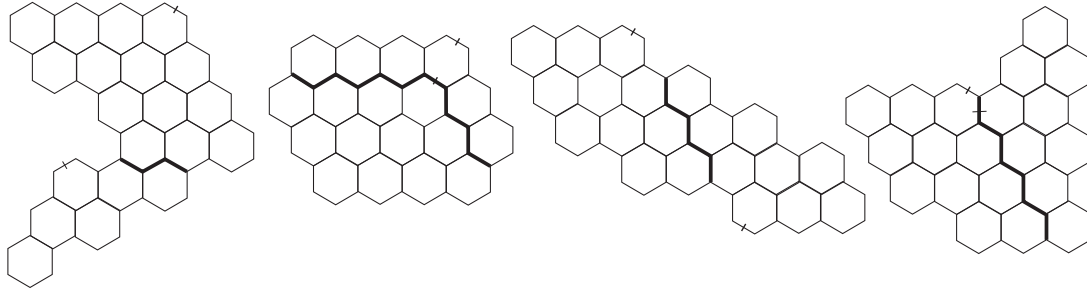


Figure 9: Four examples for gluing two truncated parallelograms along a path of odd length (marked by bold line) to get hexagonal systems with the anti-forcing number 2.

each $1 \leq i \leq m$, H_i is a linear chain with an end hexagon in H'_0 and H_i has at most many hexagons as H_{i-1} , but H_{m+1} has a hexagon adjacent left to the left end hexagon of H_m . Let s' be the right end hexagon of H_m , O' the center of s' , A' the center of the most-left vertical edge of H_m and B' the center of the edge of s' adjacent above to f_m . Then $T_2 := H \ominus e$ just lies below $A'O'B'$, and T_1 consists of H_0, H_1, \dots, H_m (see Fig. 8). So the necessity is proved.

Conversely, suppose that H is obtained from the construction that the theorem states. We can see that the anti-forcing edge e of T_1 can anti-forces all double and single edges of T_1 except for the path P . That is, $H \ominus e = T_2$. Hence $af(H) \leq 2$. Since H is not truncated parallelogram, $af(H) = 2$. \square

Finally we give some examples of applying the construction of Theorem 4.9 as shown in Fig. 9. The last graph has the minimum forcing number one. In fact, Zhang and Li [29], and Hansen and Zheng [11] determined hexagonal systems with a forcing edge. In hexagonal systems H with $af(H) \leq 2$, we can see that in addition to such kind of graphs, we always have that $af(H) = f(H)$.

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